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TO:	Ann Levine and Bruce Hope, Oregon Department of Environmental Quality (DEQ)
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DATE:	April 12, 2006
FILE:	2787-027-00
SUBJECT:	Species Sensitivity Distribution Tissue Screening Levels

The purpose of this draft memorandum is to present the summary of tissue residue toxicity (effects) data for the chemicals identified in the Statement of Work and the species sensitivity distributions (SSDs) calculated for chemicals where sufficient data was available. This memorandum is the second of two deliverables completed by GeoEngineers, Inc. (GeoEngineers) for Task Order 72-02-23 of GeoEngineers ATA contract with the DEQ.

Table 1 presents a summary of the two databases that we used to select no observed effects residue and lowest observed effects residue (NOER/LOER) data for Phase 2 of this task. Table 1 also identifies the chemicals for which a tissue screening level was calculated in Phase 1 of this task using the ambient water quality criteria and bioconcentration factor method (AWQC x BCF Method) from Sheppard, et al. (1998).

NOER/LOER DATABASE SUMMARY

DATA COMPILATION

We searched two databases to identify studies that concurrently report biological effects and whole-body residues in aquatic organisms: U.S. Army Corps of Engineers Environmental Residue Effects Database (ERED; USACE, 2005) and the U.S. Environmental Protection Agency (EPA) Office of Research and Development's effects residue database (Jarvinen and Ankley, 1999; referred to in this memorandum and associated tables as the SETAC database).

PRIMARY SCREENING CRITERIA

For each database, the number of data points for each of the chemicals is included in Table 1. Our approach to identifying useable data points for Phase 2 followed the approach recommended by Stevens et al. (2005) which included screening studies using seven primary criteria as shown below. Studies that did not meet these criteria were removed from further consideration.

- NOER/LOER concentrations had to be reported in the same study. ;
- Ecologically significant endpoints (growth, survival/mortality, and reproduction) that can be most confidently associated with ecological consequences at the population level. Endpoints included in ERED that were eliminated from consideration included behavior, biochemical, cellular, development, metabolism, morphology, and physiological effects. The SETAC database was limited to endpoints "that consist of, or are directly related to, survival, growth, and reproduction;"
- Whole body residues;
- Laboratory studies with single chemical exposures;

- Exposure route (dietary, waterborne, or maternal exposures) and duration (sufficient to equilibrate within organism);
- Measured data versus modeled; and
- Dose-dependent response demonstrated.

SECONDARY SCREENING CRITERIA

A secondary database screen was used to identify matched pairs of data (NOER/LOER) from individual studies that was not initially apparent from the information available to us in either database. In other words, because individual studies were not obtained and reviewed and some studies reported several NOER and LOER data points, it was difficult to identify which data points represented pairs from the same test. To facilitate the identification of matched pairs under this scenario, we developed and followed the secondary screening criteria as shown below. The criteria listed below represent variables that were evaluated in some or all of the tests. NOER/LOER pairs were considered as matched pairs if they came from studies where the variables were the same (e.g., the NOER and LOER were both measured in a test of 60 days using water with a pH of 7.0).

- Chemical (e.g., arsenic trioxide, disodium arsenate);
- Species;
- Life stage (e.g., adult, juvenile);
- Exposure route (e.g., ingestion, absorption);
- Review paper. Some references reported results from multiple studies;
- Study length;
- Temperature;
- Hardness of water;
- pH;
- Salinity; and
- Endpoint (e.g., prenatal mortality versus increased biomass).

Some reasons for eliminating studies from consideration under this secondary screening scenario included situations where ultraviolet light (UV-A) was applied in addition to the chemical and where the exposure route was via injection (not an ecologically relevant exposure route).

Following the secondary screen, a list of NOER/LOER pairs was identified from each database. The NOER/LOER pairs for the 18 chemicals of concern are presented electronically in the Microsoft Excel® workbook file named: SSD ERED-SETAC Database (LOER-NOER Pairs).xls. Each chemical is presented under a separate worksheet within this file.

TERTIARY SCREENING CRITERIA

The NOER/LOER pairs from each database that passed the primary and secondary screening steps were evaluated a final time in a tertiary screening step as shown below. Those NOER/LOER pairs that remained after the third screening were then used as the data set from which SSDs were generated.

- Duplicate NOER/LOER pairs were removed. The ERED and SETAC databases often both reported the same study and results.
- NOER/LOER pairs that overlapped were removed. Some of the NOER/LOER data points were reported in the SETAC database as ranges, rather than individual values. Because the unique studies were not obtained and reviewed we removed database pairs when the highest NOER was greater than lowest LOER. In cases where ranges did not overlap, the high end of the NOER range was used as the NOER and the low end of the LOER range was used as the LOER.

The NOER/LOER pairs remaining after the first two steps of the tertiary screen are shown in the second to last column of Table 1 as "Acceptable NOER/LOER Pairs."

- Finally, as presented in Stevens et al. (2005), we used NOER/LOER pairs associated with a unique species or if multiple NOER/LOER pairs were presented for a single species we calculated the geometric mean for each NOER/LOER pair and the lowest calculated geometric mean was retained. The geometric mean calculations are highlighted in the Microsoft Excel® workbook SSD ERED-SETAC Database (LOER-NOER Pairs).xls. Each chemical is presented under a separate worksheet within this file.

The NOER/LOER pairs remaining after the tertiary screen are shown in as shown in the last column of Table 1 as "Acceptable NOER/LOER Pairs (Unique Species)."

TISSUE SCREENING LEVELS – SSD METHOD

We successfully calculated SSDs for cadmium, chlordane, lead, pentachlorophenol, PCBs as Aroclors, selenium, dioxins and furans (as 2,3,7,8-TCDD), mercury, and 4,4'-DDT. SSD calculations and associated real space and natural log (ln) space graphs are included in a series of Microsoft Excel® workbooks (for example, see electronic file named "Cadmium CBCs.xls"). We generated SSDs for chemicals where there were at least four acceptable NOER/LOER pairs available based on unique species. SSDs were not calculated for arsenic, total PCBs (as 2,3,7,8-TCDD toxicity equivalents), pyrene, organic selenium tributyltin, fluoranthene, hexachlorobenzene, organic mercury, 4,4'-DDE, and 4,4'-DDD because these chemicals did not have a least four acceptable NOER/LOER pairs.

SSD CALCULATIONS

In order to calculate SSDs for each chemical, the NOER/LOER datasets were fit to the following logistic distribution model:

(Equation. 1) $P = \exp[\alpha + \beta*\ln(GM)]/[1 + \exp[\alpha + \beta*\ln(GM)]]$

Where,

- P is the cumulative proportion;
- GM is the geometric mean of the NOER and LOER; and
- Alpha (α) and beta (β) are parameters to be estimated. SYSTAT® Version 10 was used to estimate α and β for each chemical. However, SYSTAT® was unable to estimate α and β for selenium. α and β were calculated for selenium using an alternate approach described below.

The cumulative proportion was estimated by the following equation:

(Equation 2) $P = i/(n+1)$

Where,

- *i* is the rank of the GM within the data set when GMs are ordered from smallest to largest and
- *n* is the number of data points in the data set

The linear regression form of the logistic distribution model is as follows:

(Equation 3) $\text{logit}(P) = \ln[P/(1-P)] = \alpha + \beta*\ln(GM)$

Selenium

α and β were estimated for selenium using Equation 3. α and β are the intercept and slope, respectively, of the line estimated by plotting logit(P) and ln(GM) for the selenium data set. In this case, P is the cumulative proportion estimated for each data point using Equation 2 and the GM is the corresponding geometric mean. Microsoft Excel® was used to estimate α and β for selenium. The results are presented in the electronic file named "Test logistic selenium.xls".

MEAN AND CONFIDENCE BOUND CONCENTRATIONS

Mean concentrations were calculated by rearranging Equation 3 as follows:

(Equation 4) (Mean = average) $GM = \exp((\text{logit}(P)-\alpha)/\beta)$

Where,

- logit(P) = ln[P/(1-P)] where P is a chosen probability, and
- α and β were estimated as discussed above.

Confidence bound concentrations (CBCs) were calculated using the following equations as presented in *Species Sensitivity Distributions in Ecotoxicology*" (Posthuma et al., 2002). The confidence bounds on the Mean GM (in natural log space) were estimated by solving the following equation for *x* (lnGM) at a chosen *y* (P):

$$\text{(Equation 5)} \qquad \alpha + \beta * x +/- t * s * (1 + (1/n) + (x\text{-}x\text{bar})^2 / d)^{1/2}$$

Where,

- α = estimate of the intercept;
- β = estimate of the slope;
- t = critical t-value at level (1-alpha/2) with (n-2) degrees of freedom. 1-alpha is the prediction level;
- s = root mean square error from the regression model;
- *n* = number of NOER/LOER data points;
- *x*bar = average of lnGM values used for fitting the regression model;
- *d* = sum(x_i-xbar)^2; and
- *y* = logit(P) = ln[P/(1-P)].

Upper and lower confidence bounds of the GM (based on a 95% level of significance) were then calculated using the following equation:

$$\text{(Equation 6)} \qquad GM = \exp((-B +/- (B^2 - 4A*C)^{1/2}) / (2A))$$

Where,

- A = $n*d*b^2 - n*t^2*s^2$;
- B = $2*t^2*s^2*$xbar$*n - 2*b*n*d*(y-a)$; and
- C = $n*d*(y-a)^2 - t^2*s^2*(d+$xbar^2$*n)$.

SSD METHOD TISSUE SCREENING LEVELS

After calculating SSDs, we derived final tissue screening levels (TSLs) based on a specific species protection level represented by (1-P), which is chosen based on regulatory or other requirements. . As discussed in Stevens et al. (2005) and other literature, a level of 95 percent was selected as a representative species protective concentration. This upper bound is meant to protect 95 percent of all aquatic organisms that contact the chemical at this concentration. In other words 95 percent of all species that contact a chemical at

this concentration will show no adverse effects. The 95 percent species protection level corresponds to a P of 0.05.

Table 2 summarizes the TSLs that we calculated using the AWQC x BCF method and the SSD method as discussed above. For the SSD TSLs, the lower and upper confidence bounds are referred to as 95% LCL (95% lower confidence limit) and 95% UCL (95% upper confidence limit) in Table 2.

REFERENCES

Jarvinen AW, Ankley GT, 1999. Linkage of Effects to Tissue Residues: Developent of a Comprehensive Database for Aquatic Organisms Exposed to Inorganic and Organic Chemicals. Pensacola (FL), USA: SETAC Technical Publication Series. 357 p.

Posthuma L, Suter II GW, Traas TP, 2002. Species Sensitivity Distributions in Ecotoxicology. Lewis Publishers, Boca Raton, FL. pp587.

Shepard BK, 1998. Quantification of Ecological Risks to Aquatic Biota from Bioaccumulated Chemicals. National Sediment Bioaccumulation Conference Proceedings. EPA 823-R-98-002.

Stevens JA, Reiss MR, Pawlisz AV, 2005. A Methodology for Deriving Tissue Residue Benchmarks to Aquatic Biota: A Case Study for Fish Exposed to 2,3,7,8-Tetrachlorodibenzo-p-Dioxin and Equivalants. Integrated Environmental Assessment and Management; Volume 1, Number 2, p142-151.

USACE (U.S. Army Corps of Engineers), 2005. Environmental Residue Effects Database. Last Updated October 2005.

Attachments: Table 1 – NOER/LOER Databse Summary
Table 2 – Tissue Screening Levels, AWQC x BCF Method and SSD Method

Files contained on CD:
SETAC and ERED Databases (SSD ERED-SETAC Database (LOER-NOER Pairs.xls; 14 worksheets)
Confidence bound concentration workbooks (10 workbooks; 2 for selenium)
Systat Version 10 statistical output (All_Chemicals_V3.pdf).

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